Atomic and Molecular Data for Interstellar Studies: a Status Report

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Abstract

Most interstellar species have a large fraction of their electronic transitions at far ultraviolet wavelengths. Observations at these wavelengths reveal spectra rich in absorption lines seen against the continuum of a background source, such as a hot star in our Galaxy, a supernova in a nearby galaxy, or even a bright nucleus in an active galaxy. Most of the observations continue to be made with space-borne instruments, but recent work includes measurements of extragalactic material at large redshifts obtained at high resolution with large ground-based telescopes (e.g., the Keck Telescope). The combination of precise experimental oscillator strengths, large-scale computations, and astronomical spectra with high signal-to-noise ratios are yielding a set of self-consistent f-values that span a range in strength in excess of 100 for more and more species. The large range is important for studies involving the different environments probed by the various background sources. This review highlights recent work on the atomic species. Si II, S I, and Fe II, and on the molecules, CO and C_2.

1. Introduction

Two major developments in interstellar spectroscopy occurred since the 4th International Colloquium in Gaithersburg, MD. The first one involves high-resolution spectra ($\lambda/\delta\lambda \sim 100,000$) of quasars that are being acquired with the 10 meter Keck Telescope in Hawaii. One remarkable example is the detection of ultraviolet absorption lines from the fine structure levels in the ground state of C I, but observed at visible wavelengths because the intervening gas has a redshift of nearly 2 [1]. Besides the fact that very high-quality data were obtained on a faint object, these measurements provide a way of probing the cosmic background radiation temperature at a redshift of ~ 2 through an analysis of the relative populations for the fine structure levels.

The second development pertains to observations with the Goddard High Resolution Spectrograph (GHRS) on the Hubble Space Telescope. The quality of the data is outstanding; interstellar lines with peak absorption approximately 1% of the stellar continuum are routinely observed (e.g., [2–5]). Because quite high signal-to-noise ratios are being attained (typically 200 to 1000), many weak lines of interstellar species are detectable, including intercombination lines. The methods of acquiring such data are described by Cardelli and Ebbets [6], Fitzpatrick and Spitzer [7], and Lambert et al. [8]. The data quality is so high that in more and more instances the available laboratory and theoretical results on oscillator strengths are the

limiting factor in interpreting the data. The focus of our review is on this very point, where we show the importance of combining precise laboratory measurements, large-scale computations, and astronomical data from the GHRS.

The basic premise in analyzing the interstellar atomic data involves use of precise experimental f-values for multiplets containing a weak line to ensure the linearity between amount of absorption and abundance. This abundance then is used to derive a suite of self-consistent oscillator strengths for the other lines. The relative f-values derived astronomically therefore are placed on an absolute scale using precise experimental results. The final step involves comparing the astronomically-derived oscillator strengths with results from large-scale computations. As discussed below in Section 2, such comparisons probe the limitations of the calculations and can lead to improvements in the atomic structure calculations. Section 3 describes comparisons between experimental f-values, theoretical results, and astronomical results for interstellar CO and C_2.

Our review for the most part presents results not compiled previously. Another source for recent reviews is the proceedings of the international conference on high-resolution spectroscopy. These proceedings contain papers on interstellar studies [9, 10] and a paper on related GHRS results for the chemically peculiar star χ Lup [11]. In the present volume, reviews on related subjects are those by Lekrone on GHRS spectra of χ Lup and by Sonneborn on needs for the upcoming FUSE (Far Ultraviolet Spectroscopy Explorer) mission.

2. Interstellar atoms

2.1. Singly-ionized silicon and magnesium

The issue about which f-values to use in interstellar studies on Si II absorption arose in previous colloquia in the series (e.g., [12–15]). New laboratory results and recent GHRS measurements seem to be converging finally on a single set of f-values. For most lines of sight, only weak lines of Si II provide a reliable measure of the silicon abundance. Cardelli et al. [16] detected both the relatively weak allowed line at 1808 Å and the very weak intercombination line at 2335 Å. They derived column densities for Si II that differed by less than 10% when the recent laboratory results for λ 1808 [17] and λ 2335 [18] were used in the analysis. The experimental

work on λ 1808 also provided confirmation of the large-scale theoretical results of Dufton *et al.* [19]. Spitzer and Fitzpatrick [20], who studied the low density sight line to HD 93125, used the results of Dufton *et al.* for λ 1808 to obtain self-consistent column densities from the lines at 1304 and 1527 Å. Their analysis suggested that $f_{1304} = 8.6 \times 10^{-2}$ and $f_{1527} = 1.10 \times 10^{-1}$, values that agree remarkably well with the large-scale theoretical work of Hibbert *et al.* [21] — 8.8×10^{-2} and 1.30×10^{-1}, respectively. Hibbert *et al.* predicted a lifetime of 0.904 ns for the upper state involved in λ 1527; a new beam-foil study (Schectman, private communication) confirms this prediction. Thus, the situation for Si II *f*-values is much improved from just a few years ago.

On the other hand, interstellar Mg abundances are still not well defined because the *f*-value for the weak doublet of Mg II near 1240 Å is not known to better than a factor of 5. As noted by Sofia *et al.* [22], this line is the best one for obtaining reliable abundances for Mg, but the analyses are hindered by the uncertain *f*-value. Since it appears that the expected lifetimes are beyond the capabilities of present experimental techniques, additional large-scale computations are necessary for this ion.

2.2. Neutral sulfur

Federman and Cardelli [23] detected 27 lines of S I arising from 14 multiplets toward ζ Oph. The absorption comes from the velocity component associated with dense gas ($v_{\text{helio}} = -15 \text{ km s}^{-1}$) because neutral sulfur, like other atoms whose ionization potential is less than hydrogen's, is a minor constituent. In a direction with a single principal component, a curve of growth can be used to extract the abundance of S I from a weak line of a multiplet and the Doppler width (or *b*-value) for the absorbing material from a strong line of the multiplet.

The curve of growth for S I was based on precise experimental *f*-values [24, 25]. The analysis started with a determination of the S I column density and associated *b*-value from the multiplet at 1479 Å. The *f*-values for the other lines then were adjusted so that a single column density and *b*-value described the data. The uncertainties in the astronomically derived *f*-values range from 10% to 20%. In all cases, *LS* coupling was assumed to apply for the derivation of multiplet oscillator strengths; Beideck *et al.* [25] found this to be the case in their measurements of the multiplets λλ 1814, 1299. Unlike most previous interstellar studies using the curve-of-growth method, several lines detected with the

GHRS have optical depths at line center less than 0.5: these weak lines are essential for an accurate and unambiguous curve of growth.

The astronomically derived S I *f*-values are compared with other determinations in Tables I and II. Of particular interest is the comparison with the results from the Opacity Project [27]. In this comparison keep in mind that the astronomical values have uncertainties of 10–20%. Table I shows that our results for transitions involving the ground state of S I ($3p^4 \, ^3P$) and excited $^3S^0$ and $^3P^0$ states agree with the theoretical results from the Opacity Project at the 5–10% level! Furthermore, the interstellar results reveal no discernible difference with the experimental work of Beideck *et al.* [25] for the multiplets λλ 1814, 1299. The results for the $^3D^0$ states are not always as consistent (see Table II), but where significant disagreement arises (~50% level), the differences can be traced to additional mixing among levels beyond what was considered in the calculations. In particular, $^3D^0$ states having an excited core need to be included: Mixing occurs between $3p^3(^4S^0)3d \, ^3D^0$ and $3p^3(^2D^0)4s' \, ^3D^0$ and between $3p^3(^2D^0)3d \, ^3D^0$ and both $3p^3(^4S^0)5d \, ^3D^0$ and $3p^3(^4S^0)6d \, ^3D^0$ [28]. Hibbert (private communication) is now examining this issue through detailed calculations.

2.3. Singly-ionized iron

Unlike S I, Fe II is the dominant form of iron in interstellar space and absorption is seen in many components. As a result, Fe II probes many kinds of interstellar environments and is, therefore, a guide to metal enrichment/depletion. Curves of growth are usually not reliable under such circumstances and another method is needed to analyze the data. Cardelli and Savage [29] studied the observed variation of apparent optical depth with velocity (the $\tau - v$ method) for Fe II lines. The $\tau - v$ method allows one to express the apparent column density at each data point in velocity. Comparison between weak (small *f*-value) and strong (large *f*-value) lines can be used to check for unresolved saturated structure in the cores of the stronger lines. In the limit where no unresolved saturation is present, the apparent column density profiles for weak and strong lines match each other.

The determination of *f*-values utilized two relatively weak transitions of Fe II for which new accurate laboratory *f*-values [30] are available to place the analysis on an absolute basis. Through use of the apparent column density method, comparisons between these transitions and others (both weaker and stronger ones) allowed Cardelli and

Table I. *Comparison of oscillator strengths involving $^3S^0$ and $^3P^0$ states of neutral sulfur*

Multiplet Wavelength (Å)	Designation	*f*(FC)[a]	*f*(exp)[b]	*f*(MZ)[c]	*f*(BMZ)[d]
1814	4s $^3S^0$	8.8×10^{-2}	$(8.8 \pm 0.5) \times 10^{-2}$	8.5×10^{-2}	9.2×10^{-2}
1405	5s $^3S^0$	1.43×10^{-2}	—	1.2×10^{-2}	1.5×10^{-2}
1307	6s $^3S^0$	5.04×10^{-3}	—	4.0×10^{-3}	4.8×10^{-3}
1299	4s″ $^3P^0$	1.21×10^{-1}	$(1.21 \pm 0.04) \times 10^{-1}$	1.16×10^{-1}	1.18×10^{-1}
1266	7s $^3S^0$	2.59×10^{-3}	—	2.0×10^{-3}	2.1×10^{-3}
1245	8s $^3S^0$	1.06×10^{-3}	—	—	1.1×10^{-3}

[a] From [23]. Typical uncertainties range from 10% to 20%. For the multiplets with strong lines (λλ 1814, 1299), there are no discernible differences with the experimental results of Beideck *et al.* [25].
[b] Experimental results from [25].
[c] From [26].
[d] Opacity Project results from [27].

Table II. *Comparison of oscillator strengths involving $^3D^0$ states of neutral sulfur*

Multiplet Wavelength (Å)	Designation	f(FC)[a]	f(exp)[b]	f(MZ)[c]	f(BMZ)[d]
1479	$4s'\,^3D^0$	9.9×10^{-2}	$(9.9 \pm 0.8) \times 10^{-2}$	2.1×10^{-2}	4.3×10^{-2}
1429	$3d\,^3D^0$	1.68×10^{-1}	$(1.49 \pm 0.11) \times 10^{-1}$	1.72×10^{-1}	1.51×10^{-1}
1320	$4d\,^3D^0$	4.52×10^{-2}	—	2.6×10^{-2}	2.8×10^{-2}
1274	$5d\,^3D^0$	1.08×10^{-2}	—	2.0×10^{-3}	4.3×10^{-3}
1256	$6d\,^3D^0$	1.92×10^{-3}	—	—	9.2×10^{-5}
1227	$8d\,^3D^0$	$\leqslant 1.2 \times 10^{-3}$	—	—	1.3×10^{-3}

[a] From [23]. Typical uncertainties range from 10% to 20%. The analysis was based on the experimental results for λ 1479.
[b] Experimental results from [24, 25], where the relative f-values of Doering [24] were combined with the results of Beideck et al. [25] for λ 1814.
[c] From [26].
[d] Opacity Project results from [27].

Savage to determine corrections to the existing f-values since by definition, all transitions should yield the same apparent column density in the limit of no unresolved saturated structure. In all, f-values for 9 transitions of Fe II, spanning a range in absorption strength of over a factor 4000, were analyzed. A composite apparent column density profile for Fe II toward β^1 Sco was constructed by combining portions of different profiles where there is no unresolved saturated structure. The resulting apparent column density profile is remarkable in that it shows Fe II column densities spanning a range of 10 000 in a single sight line.

The astronomical results for Fe II are timely. They provide a benchmark for comparison with the ongoing work of the Iron Project. For transitions that do not involve a spin change, the available results from the Iron Project [32] for strong lines agree nicely (at the 15% level) with the astronomical results, but the correspondence is not very good for the weakest lines (see Table III). The differences for the weak lines may be attributed to the fact that the theoretical calculations could be providing a poorer representation for some of the highly excited states. The results in Morton's compilation [31] are also shown in Table III. For lines with $f \geqslant 10^{-2}$, there is quite good agreement, but again the correspondence worsens for weaker lines. These comparisons highlight the importance of high-quality astronomical data on weak lines from GHRS. The amount of Fe II in a variety of interstellar environments is more clearly defined than was possible in the past, and these results will be useful in placing analyses of QSO absorption systems, including those at high redshift studied with the Keck Telescope, on a firmer foundation. Further improvements can be expected from ongoing laboratory work (see poster by Bergeson et al.).

2.4. Elements heavier than zinc

The synthesis of elements heavier than Zn differs appreciably from the synthesis of the lighter elements (e.g., [33]). The incorporation of helium nuclei dominates for Zn and lighter elements, while neutron capture is important for the heavier elements. Until the launch of the Hubble Space Telescope, there was no direct information on the abundances of the heavy elements in interstellar space. Spectra from GHRS yielded detections of absorption from Ga, Ge, As, Se, Kr, Cd, Sn, Tl, and Pb [2, 4, 34–36]. In all cases, strong resonance lines of the dominant ion were seen.

Although resonance lines are measured, the analysis of abundance is hindered by the small number of precise oscillator strengths. Most of the theoretical results use a limited set of configurations and most available experimental results are only accurate to 20–30%. The situation is improving on the theoretical side: Brage and Leckrone [37] obtained results for As II based on a large-scale computation, and Brage and colleagues presented a poster at this colloquium on f-values for Tl II. As pointed out in the poster by

Table III. *Comparison of oscillator strengths for singly ionized iron*

Line Wavelength (Å)	Upper State[a]	f(CS)[b]	f(M)[c]	f(N)[d]
1142	$y\,^6F^0_{7/2}$	$(2.47 \pm 0.32) \times 10^{-3}$	$(5.00 \pm 1.75) \times 10^{-3}$	1.65×10^{-3}
1608	$y\,^6P^0_{7/2}$	$(6.19 \pm 0.62) \times 10^{-2}$	$(6.19 \pm 1.86) \times 10^{-2}$	8.92×10^{-2}
1611	$y\,^4F^0_{7/2}$	$(1.02 \pm 0.14) \times 10^{-3}$	2.22×10^{-4}	—
2249	$z\,^4D^0_{7/2}$	$(1.82 \pm 0.14) \times 10^{-3}$	$(2.51 \pm 0.22) \times 10^{-3}$	—
2261	$z\,^4F^0_{9/2}$	$(2.44 \pm 0.19) \times 10^{-3}$	$(3.72 \pm 0.73) \times 10^{-3}$	—
2344	$z\,^6P^0_{7/2}$	$(1.10 \pm 0.08) \times 10^{-1}$	$(1.10 \pm 0.08) \times 10^{-1}$	1.26×10^{-1}
2368	$z\,^6F^0_{7/2}$	$(6.28 \pm 1.13) \times 10^{-5}$	$(1.60 \pm 0.11) \times 10^{-4}$	4.25×10^{-3}
2374	$z\,^6F^0_{9/2}$	$(3.26 \pm 0.23) \times 10^{-2}$	$(2.82 \pm 0.20) \times 10^{-2}$	5.27×10^{-2}
2383	$z\,^6F^0_{11/2}$	$(3.00 \pm 0.21) \times 10^{-1}$	$(3.00 \pm 0.21) \times 10^{-1}$	3.43×10^{-1}
2587	$z\,^6D^0_{7/2}$	$(6.84 \pm 0.55) \times 10^{-2}$	$(6.46 \pm 0.45) \times 10^{-2}$	5.48×10^{-2}
2600	$z\,^6D^0_{9/2}$	$(2.13 \pm 0.18) \times 10^{-1}$	$(2.24 \pm 0.16) \times 10^{-1}$	2.40×10^{-1}

[a] Ground state is $4s\,^6D_{9/2}$.
[b] From [29], which is based on the f-values of Bergerson et al. [30] for $\lambda\lambda$ 2249, 2261.
[c] Morton's compilation [31].
[d] Iron Project results from [32].

Morton, experimental data are needed for most of these heavy elements.

3. Interstellar molecules

3.1. *Carbon monoxide*

Carbon monoxide (CO) is the second most abundant molecule in interstellar space. Ultraviolet data obtained with the Hubble Space Telescope yield high-quality spectra showing many bands of the A–X system (e.g., [8]). In order to extract the most reliable abundances, one is interested in the weakest, optically thin bands ($v' \geqslant 7$). Unfortunately, the available information on oscillator strengths for these bands spans a range of 20–30%, which is larger than the uncertainties associated with the astronomical measurements. Table IV shows the comparison of results. The theoretical results of Kirby and Cooper [38] and experimental determinations using electron-energy-loss spectroscopy [39–41] agree nicely, as do absorption measurements for $v' = 11$–14 [42]. Another absorption experiment [43], however, reported results that are consistently 20–30% larger than the others. The cause for the difference is difficult to ascertain because for the bands with $v' \leqslant 6$ for which optically thick absorption complicates the data analysis, all results agree at the 5–10% level. The astronomical measurements of Lambert *et al.* [8] seem most consistent with the results of Chan *et al.* [41]. Federman and colleagues are attempting to understand the reason for the different results through new absorption measurements of the A–X system of bands acquired at the Synchrotron Radiation Center of the University of Wisconsin-Madison. Through the use of a short gas cell (2.6 mm) and low pressures, complications related to optically thick lines should be minimized. Moreover, another electron-energy-loss experiment (Mason, private communication) was completed recently and another absorption experiment is planned by Eidelsberg and collaborators (Rostas, private communication). The goal of course is to reach consensus on a set of f-values to use.

Weak bands from triplet-singlet transitions are also found in GHRS spectra [5]. The situation for extracting a CO abundance from these data was reviewed by Federman [10]. There appears to be a need to improve the spectroscopically derived f-values (see [44] and references therein) for the d–X (12-0) and (5-0) bands, as well as the e–X (5-0) and (4-0) bands, because they differ in a significant way from the f-values inferred from the astronomical observations. Experiments to measure oscillator strengths directly are in the planning stages (Smith, private communication; Rostas, private communication).

Finally, we note that there is also a lack of consensus regarding the appropriate f-value to use for transitions involving Rydberg states. The situation is presented in Table V. Here, the various electron-energy-loss experiments [39, 41, 45] do not agree with each other, nor with the absorption measurements [46, 47]. The large number of lifetime measurements are not included in the comparison because they are dependent on the branching fraction used in the analysis. Since Kirby and Cooper [38] caution that their theoretical results are of limited accuracy for these transitions, their results are not included in Table V either. The lack of agreement in Table V affects the determination

Table IV. *Comparison of oscillator strengths for the CO $A\ ^1\Pi - X\ ^1\Sigma^+$ bands*

Band	f(KC)[a]	f(ERBT)[b]	f(LS/ML)[c]	f(CCB)[d]	f(SSYI)[e]
1-0	3.2×10^{-2}	$(3.4 \pm 0.3) \times 10^{-2}$	$(4.9 \pm 0.4) \times 10^{-2}$	$(3.5 \pm 0.2) \times 10^{-2}$	—
2-0	3.7×10^{-2}	$(4.2 \pm 0.4) \times 10^{-2}$	$(4.5 \pm 0.5) \times 10^{-2}$	$(4.0 \pm 0.2) \times 10^{-2}$	—
3-0	3.1×10^{-2}	$(3.8 \pm 0.4) \times 10^{-2}$	$(3.6 \pm 0.2) \times 10^{-2}$	$(3.5 \pm 0.2) \times 10^{-2}$	—
4-0	2.2×10^{-2}	$(2.6 \pm 0.3) \times 10^{-2}$	$(2.5 \pm 0.1) \times 10^{-2}$	$(2.4 \pm 0.1) \times 10^{-2}$	—
5-0	1.4×10^{-2}	$(1.6 \pm 0.2) \times 10^{-2}$	$(1.6 \pm 0.1) \times 10^{-2}$	$(1.5 \pm 0.1) \times 10^{-2}$	—
6-0	7.5×10^{-3}	$(1.0 \pm 0.1) \times 10^{-2}$	$(8.5 \pm 0.4) \times 10^{-3}$	$(8.1 \pm 0.4) \times 10^{-3}$	—
7-0	3.9×10^{-3}	$(5.6 \pm 0.6) \times 10^{-3}$	$(4.4 \pm 0.2) \times 10^{-3}$	$(4.1 \pm 0.2) \times 10^{-3}$	—
8-0	1.9×10^{-3}	$(2.9 \pm 0.3) \times 10^{-3}$	$(2.2 \pm 0.1) \times 10^{-3}$	$(2.0 \pm 0.1) \times 10^{-3}$	—
9-0	9.3×10^{-4}	$(1.4 \pm 0.2) \times 10^{-3}$	$(1.1 \pm 0.1) \times 10^{-3}$	$(9.5 \pm 0.9) \times 10^{-4}$	—
10-0	4.3×10^{-4}	$(6.5 \pm 0.7) \times 10^{-4}$	$(5.0 \pm 0.3) \times 10^{-4}$	$(4.1 \pm 0.4) \times 10^{-4}$	—
11-0	1.9×10^{-4}	$(2.8 \pm 0.3) \times 10^{-4}$	$(2.5 \pm 0.1) \times 10^{-4}$	$(1.8 \pm 0.2) \times 10^{-4}$	$(1.7 \pm 0.3) \times 10^{-4}$
12-0	8.3×10^{-5}	$(1.3 \pm 0.2) \times 10^{-4}$	$(1.0 \pm 0.1) \times 10^{-4}$	$(9.0 \pm 1.0) \times 10^{-5}$	$(6.9 \pm 0.8) \times 10^{-5}$

[a] From [38].
[b] From [43].
[c] From [39, 40].
[d] From [41].
[e] From [42].

Table V. *Comparison of oscillator strengths for (0–0) bands of other CO transitions*

Transition	f(LS)[a] $\times 10^2$	f(EBVR)[b] $\times 10^2$	f(CCB)[c] $\times 10^2$	f(KJA)[d] $\times 10^2$	f(SSIY)[e] $\times 10^2$
$B\ ^1\Sigma^+ - X\ ^1\Sigma^+$	1.53 ± 0.14	0.452 ± 0.045	0.803	1.2 ± 0.3	—
$C\ ^1\Sigma^+ - X\ ^1\Sigma^+$	16.3 ± 1.5	6.19 ± 0.62	11.77	15.4 ± 4.1	—
$E\ ^1\Pi - X\ ^1\Sigma^+$	9.4 ± 0.9	3.65 ± 0.37	7.06	—	4.9 ± 0.5

[a] From [39].
[b] From [46].
[c] From [41].
[d] From [45].
[e] From [47].

of the photodissociation rate for CO because these Rydberg transitions play an important role in the process (see [48]).

3.2. *Molecular carbon*

A new experiment [49] seems to have cleared up the discrepancy for the A–X (2-0) band of C_2 noted by Lambert *et al.* [50] and discussed in a review [10]. The theoretical *f*-value of Langhoff *et al.* [51] – 1.44×10^{-3}, the astronomical one derived by Lambert *et al.* [50] – $(1.23 \pm 0.16) \times 10^{-3}$, and the experimental one – $(1.36 \pm 0.15) \times 10^{-3}$ – are now in excellent agreement. According to Erman and Iwamae [49], the differences with previous measurements arose because a redistribution among stages through collisions took place. In particular, the buffer gas appears to have induced transfers between the A state and the B' and/or B state.

4. Concluding remarks

Since the 4th Colloquium, GHRS spectra, in combination with precise laboratory measurements and large-scale calculations, have led to self-consistent sets of oscillator strengths for a number of interstellar species. In this review we highlighted the results for S II, S I, Fe II, and C_2. We also showed that more work on Mg II and CO is needed and that precise experimental *f*-values are required for analyses of many heavy elements.

We end this review by noting the directions our new GHRS spectra are leading us. Many new interstellar lines of Ni II are seen in our spectra. A self-consistent set of oscillator strengths is the objective for this analysis, thereby providing an empirical test for the theoretical work of Kurucz (see [31]). There is also a large number of lines from the three fine structure levels for C I. Since the results from different lines must be self-consistent, our high-quality data can lead to an improved set of *f*-values for this species also.

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